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Title: The Search For Thermodynamic Principles of Organization

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The Search for Thermodynamic Principles of Organization

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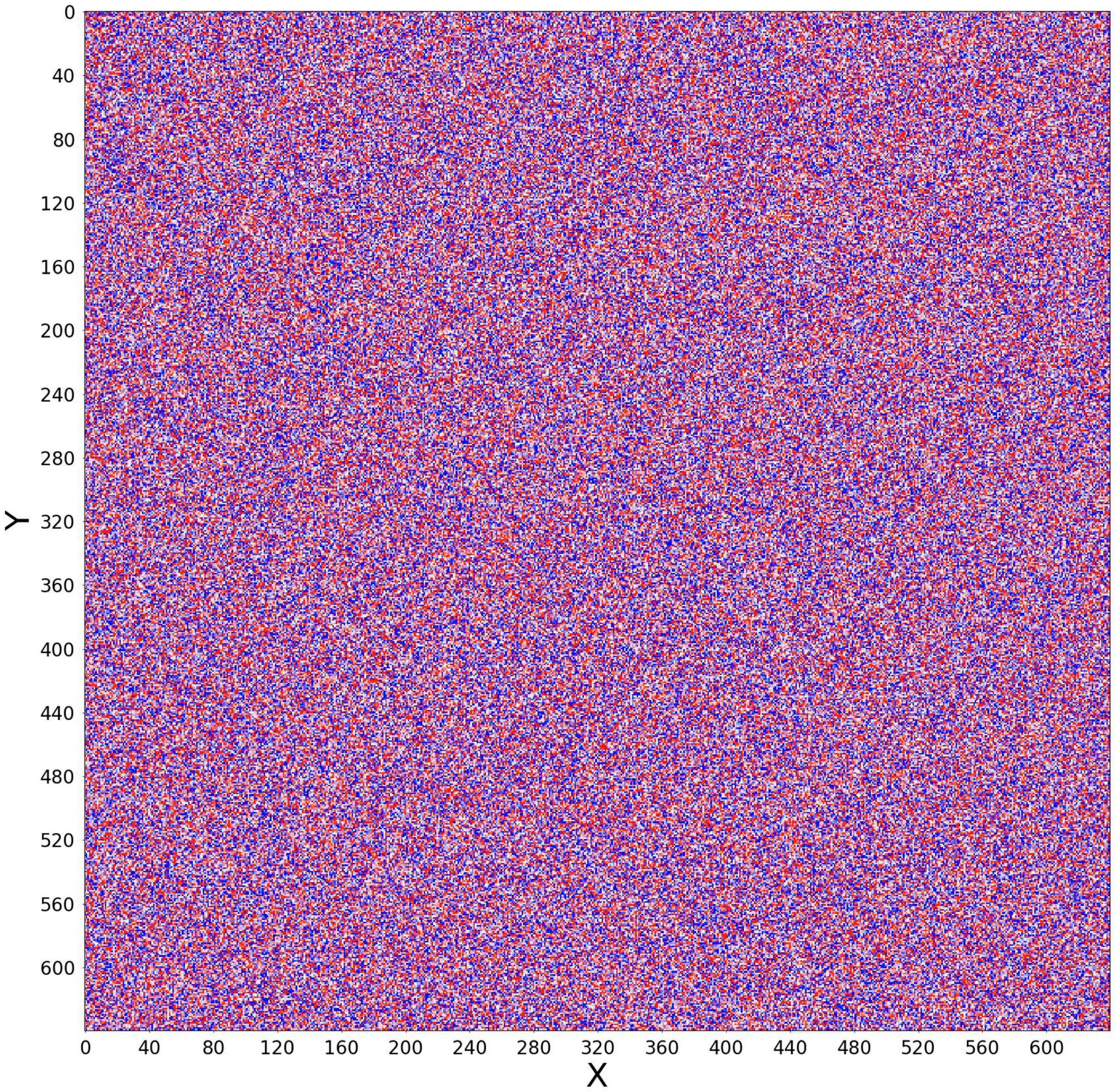
Example: vortex gas

$$\zeta_t + \psi_x \zeta_y - \psi_y \zeta_x = \nu \nabla^2 \zeta$$

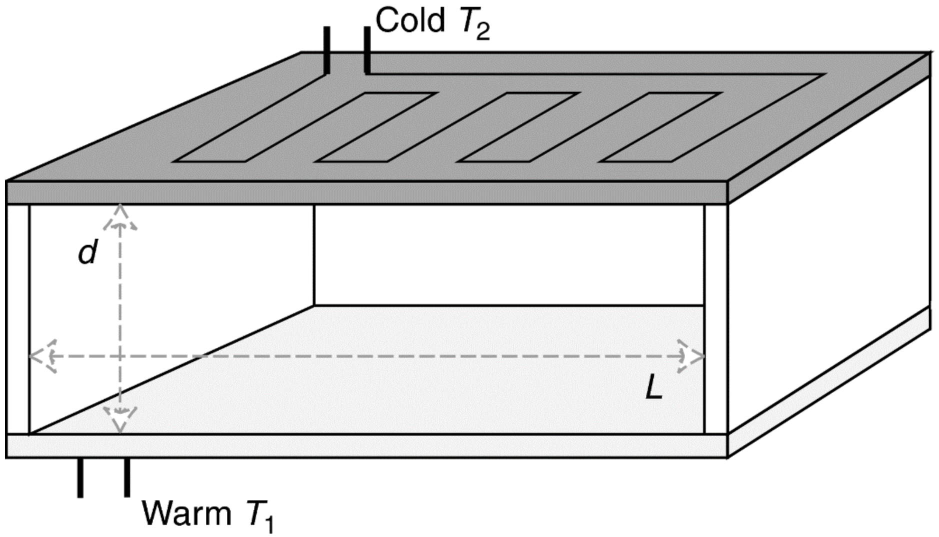
$$\zeta = \mathbf{v}_x - \mathbf{u}_y = \nabla^2 \psi$$

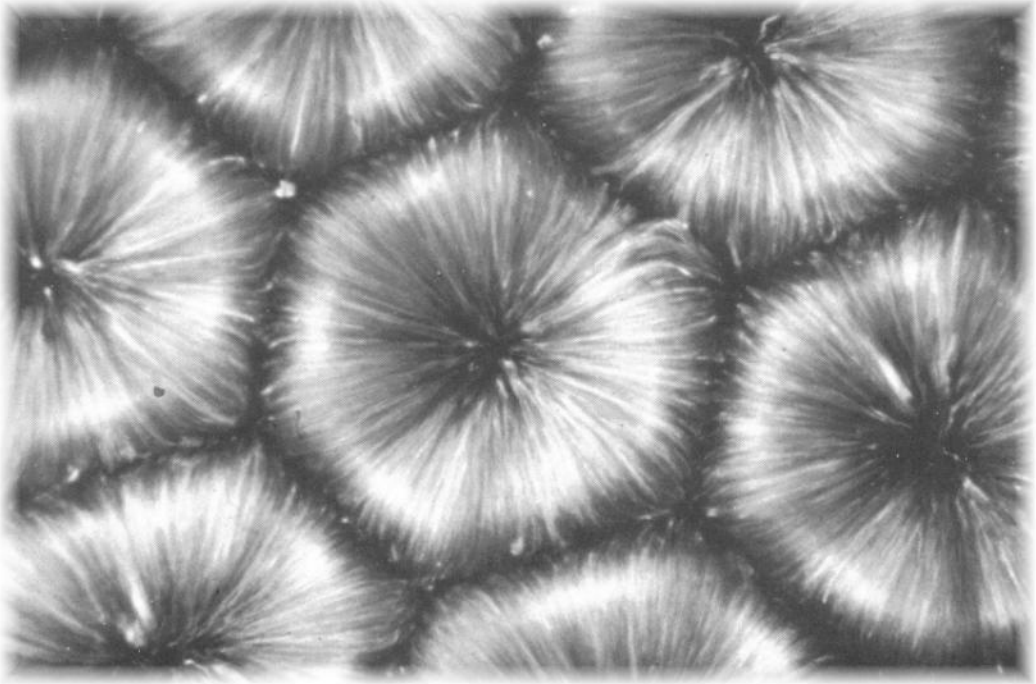


Overview

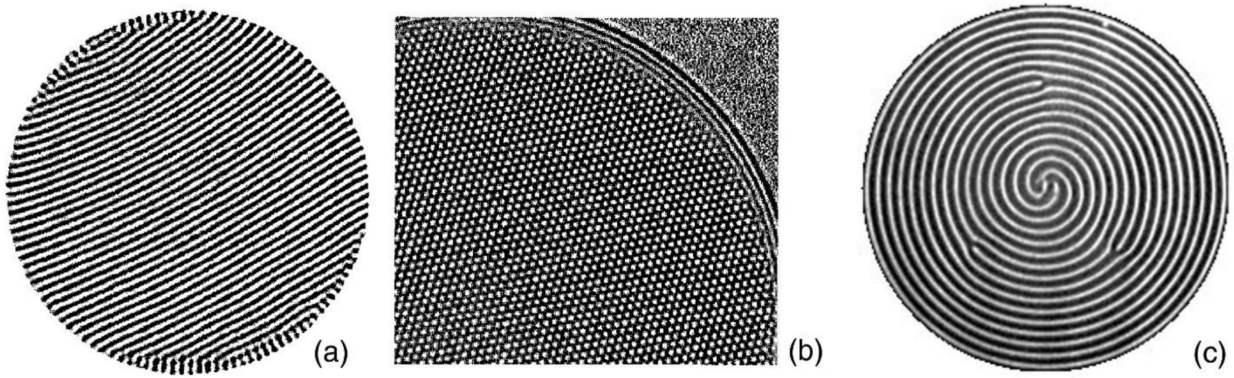
- Stability analysis and selection principles
  - Nonlinear dynamics
  - Equilibrium thermo
  - Nonequilibrium thermo
- Formalizing organization
  - Organization as intrinsic computation: causal states
  - Modes of organization: transfer operators
- Nonequilibrium statistical mechanics of organization
  - Partially-observed systems
  - Connecting causal states and transfer operators with Mori-Zwanzig formalism

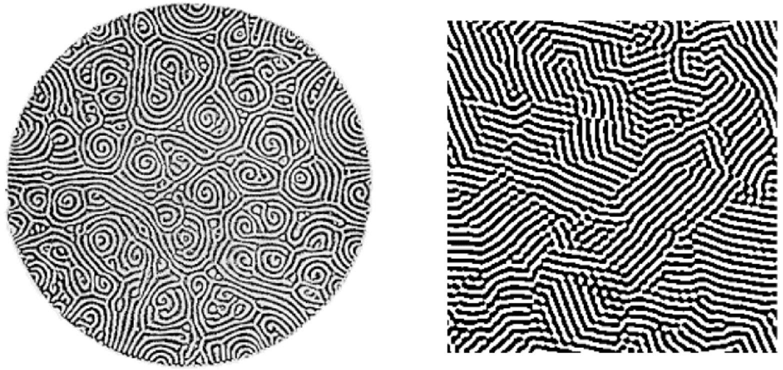
Example: Rayleigh-Bénard Convection





M. Van Dyke. *An Album of Fluid Motion*. Parabolic Press





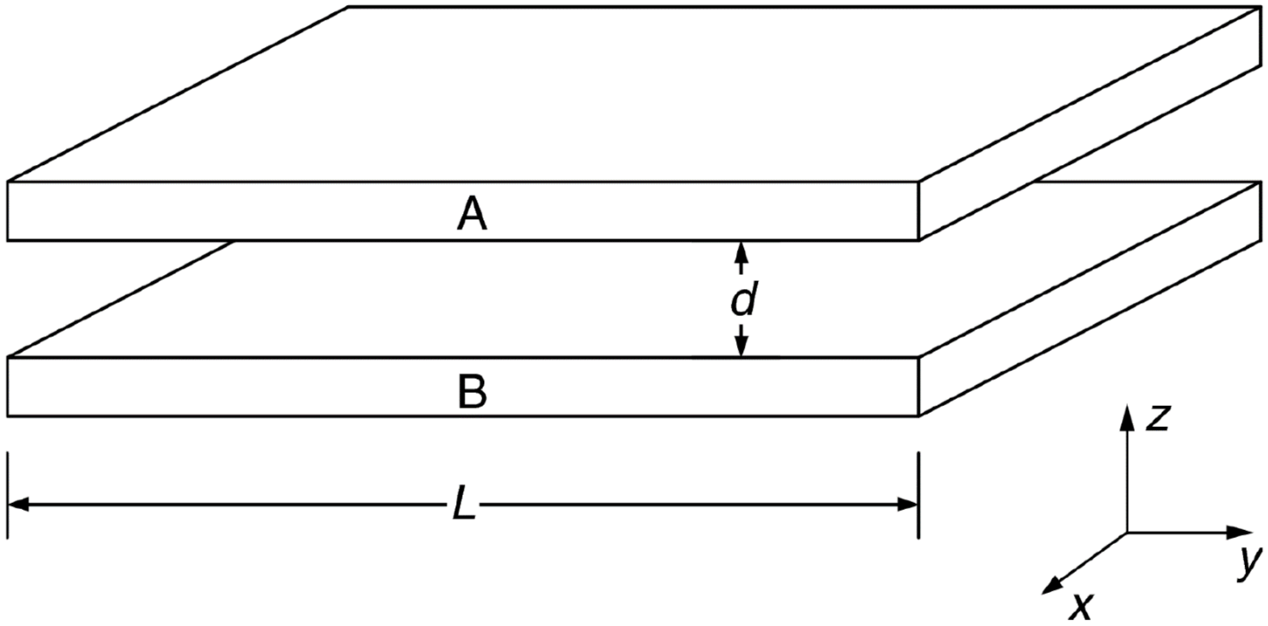
Images: David Cannell, University of California at Santa Barbara

(a) (b)

Conceptual Framework: Patterns Near Equilibrium

- Gradients in intensive quantities drive fluxes in extensive quantities
- Bifurcation parameter $R \propto \frac{\text{driving}}{\text{dissipation}}$ = "distance from equilibrium"

- *Equilibrium*: $R = 0$
  maximal symmetry
- *Base state*: $0 < R < R_c$
  symmetry broken along gradient
- *Patterned state*: R just above R_c
  - *Primary bifurcation*



Nonlinear Dynamics: Bifurcation Theory

- $\partial_t X(r,t) = F\big(X(r,t), \partial_r X(r,t), \ldots; R\big)$
- Steady-state $\partial_t X^*(r,t) = 0$ unstable at R_c
- Growing perturbation $\delta X(r,t) = Ae^{\sigma t}e^{ik_c \cdot r}$ saturates to create patterned state

Rayleigh-Bénard Convection

- Navier-Stokes + heat conduction+ *constitutive relations*
- Thermo: closed top (buoyancy) vs open top (surface-tension)

M. F. Schatz, S. J. VanHook, W. D. McCormick, J.B. Swift, and H. L. Swinney. Onset of surface-tension-driven Benard convection. Physical review letters, 75(10):1938, 1995.

- Rayleigh R_c calculation: density varies with temp, no surface tension effects

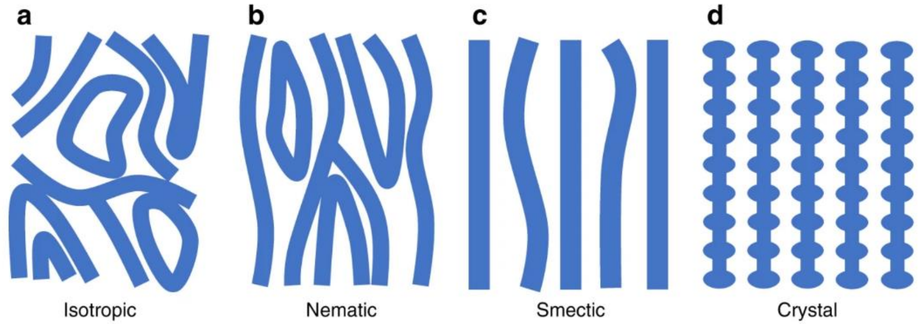
Lord Rayleigh. On convection currents in a horizontal layer of fluid, when the higher temperature is on the under side. Phil. Mag. (Series 6), 32(192):529-546, 1916.

- Pearson R_c calculation: surface tension varies with temp, no density effects

J.R.A. Pearson. On convection cells induced by surface tension. Journal of fluid mechanics, 4(5):489-500, 1958.

Equilibrium Thermo and The 2^{nd} Law

- Spontaneous self-organization not in conflict with 2^{nd} Law
  A. T. Winfree, The prehistory of the Belousov-Zhabotinsky oscillator. *Journal of Chemical Education*, (61)8:661, 1984
- Entropy is *not* measure of disorder!
  A. Ben-Naim, A Farewell to Entropy: Statistical Thermodynamics Based on Information: S. World Scientific, 2008.
  W. T. Grandy Jr. Entropy and the time evolution of macroscopic systems. Vol.141. Oxford, 2008.
- Organization in Equilibrium: $F = U - TS$
  - e.g. strongly-correlated electron systems, liquid crystals



Q. Qian, J. Nakamura, S. Fallahi, G. C. Gardner & M. J. Manfra, Possible nematic to smectic phase transition in a two-dimensional electron gas at half-filling. N Comms (2017)

- Classical Irreversible Thermo: $dS = d_eS + d_iS,$ $\boxed{d_iS \geq 0,}$ (e.g) $d_eS = \frac{dQ}{T}$
  entropy production
  - Reversible process: $d_iS = 0 \implies dS = \frac{dQ}{T}$
  - 2^{nd} Law: $d_eS = 0 \implies dS \geq 0$

Nonequilibrium Thermo: Theory of Dissipative Structures

- Thermodynamic (entropic) stability theory proposed by Prigogine et al
  P. Glansdorff and I. Prigogine. Thermodynamic theory of structure, stability and fuctuations. Willey, 1971.
  G. Nicolis and I. Prigogine. Self-Organization in Nonequilibrium Systems. Wiley, New York, 1977.
- Argued for Minimum Entropy Production Principle
  $\Longrightarrow$ Base state always stable $\Longrightarrow$ No organization near equilibrium
- "Universal Evolution Criteria" — *excess entropy production* as Lyapunov function
  - determines stability far from equilibrium

- Neither of the above appear to hold in general
  - No universally accepted (near equilibrium) steady-state variational principle
    R. Landauer. Inadequacy of entropy and entropy derivatives in characterizing the steady state. Physical Review A, 12(2):636, 1975.
    E. T. Jaynes. The minimum entropy production principle. Ann. Rev. Phys. Chem., 31:579-601, 1980.
    W. T. Grandy Jr. Entropy and the time evolution of macroscopic systems. Vol.141. Oxford, 2008.
  - Excess entropy production does not determine stability
    J. Keizer and R.F. Fox. Qualms regarding the range of validity of the glansdorff-prigogine criterion for stability of non-equilibrium states. PNAS, 1974.
    R.F. Fox. The "excess entropy" around nonequilibrium steady states, $(\delta^2 S)_{ss}$, is not a liapunov function. PNAS, 1980.

Organization and Intrinsic Computation

- For stochastic process $\{X_t\}$:
  - *past* at time t is $\overleftarrow{x}_t = \{x_t, x_{t-1}, x_{t-2}, \ldots\}$; *future* is $\overrightarrow{x}_t = \{x_{t+1}, x_{t+2}, \ldots\}$
- *causal states* defined as equivalence classes of

$$\overleftarrow{x}_i \sim_\epsilon \overleftarrow{x}_j \iff \Pr(\overrightarrow{X} | \overleftarrow{x}_i) = \Pr(\overrightarrow{X} | \overleftarrow{x}_j)$$

- Dynamics governed by *semigroup* of Markov operators generated by

$$S_{t+1} = M_\epsilon S_t$$

with $M_\epsilon^t (M_\epsilon^{t'} S) = M_\epsilon^{t+t'} S \qquad t, t' \in N^+$

- Semigroup algebra formalizes pattern / organization as generalized symmetries

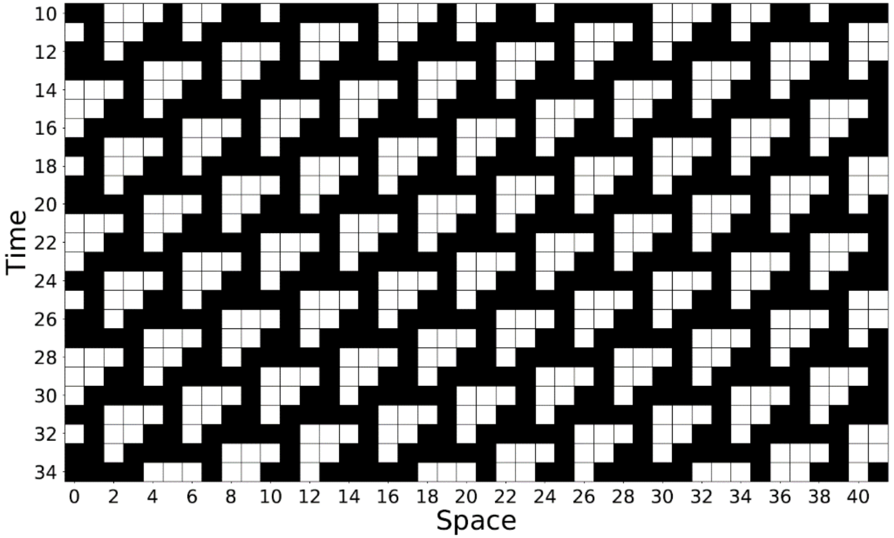
A. Rupe, A Behavior-Driven Theory of Emergent Pattern and Structure in Complex Spatiotemporal Systems. PhD Dissertation, UC Davis (2020)
A. Rupe and J. P. Crutchfield, An Algebraic Theory of Patterns as Generalized Symmetries, in progress (2021)

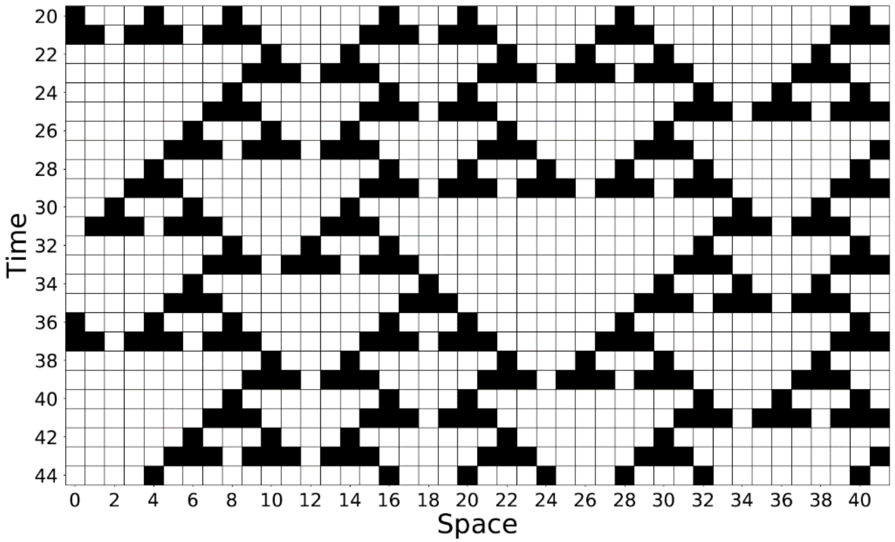
Explicit Symmetry

Hidden Symmetry

Observable Fields

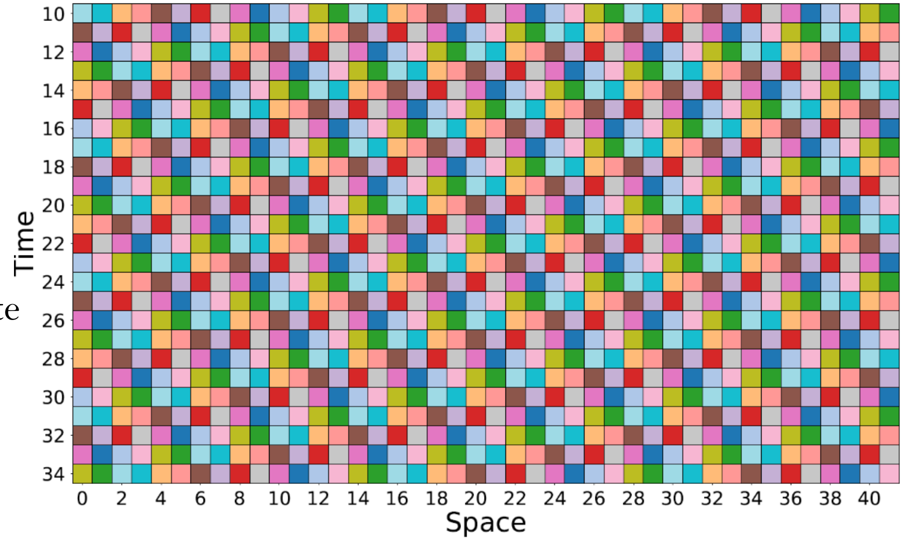
white = 0
black = 1

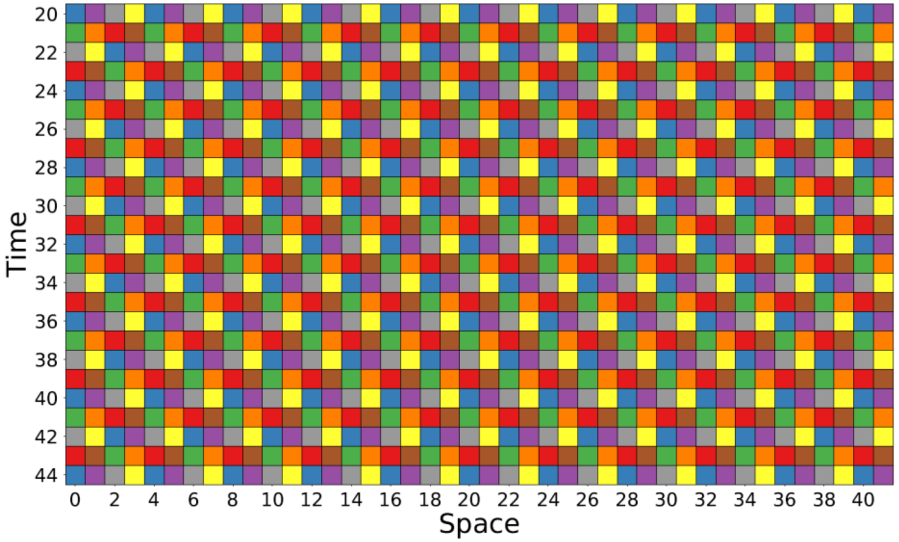




Latent Fields

unique color = unique state
(equiv. class of past LCs)





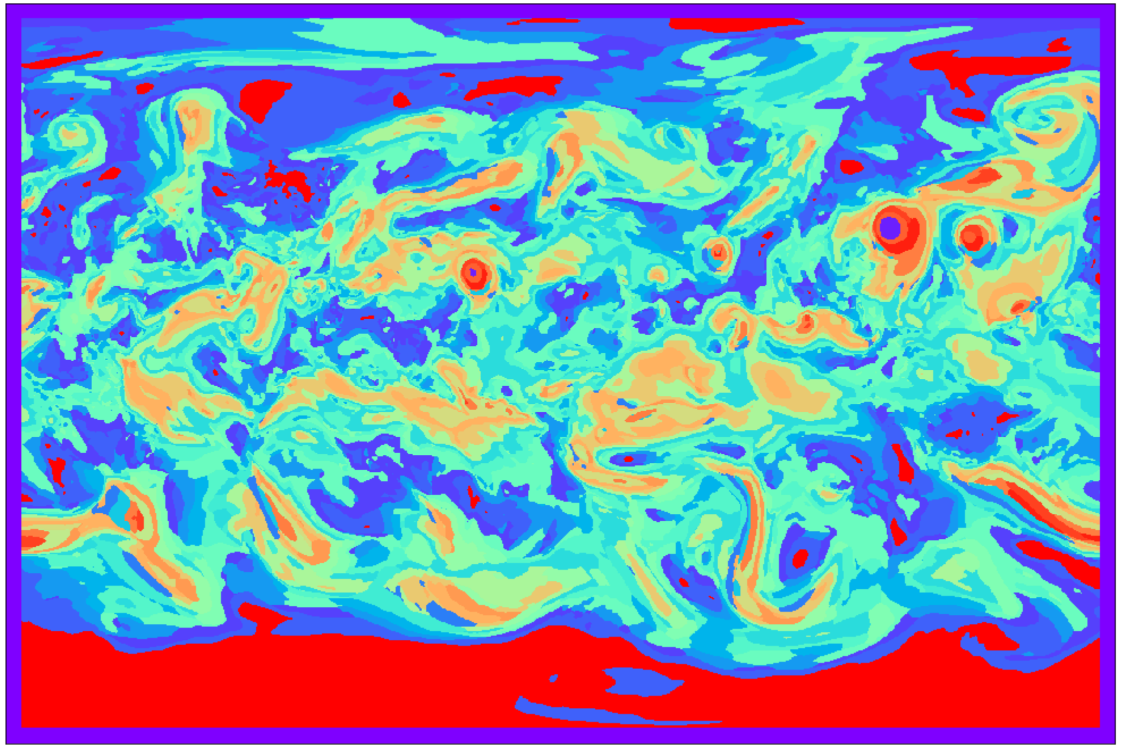
A. Rupe and J. P. Crutchfield, "Local Causal States and Discrete Coherent Structures". Chaos: An Interdisciplinary Journal of Nonlinear Science 28:7, 075312 (2018)
A. Rupe and J. P. Crutchfield, "Spacetime Symmetries, Invariant Sets, and Additive Sub-Dynamics of Cellular Automata", arXiv:1812.11597

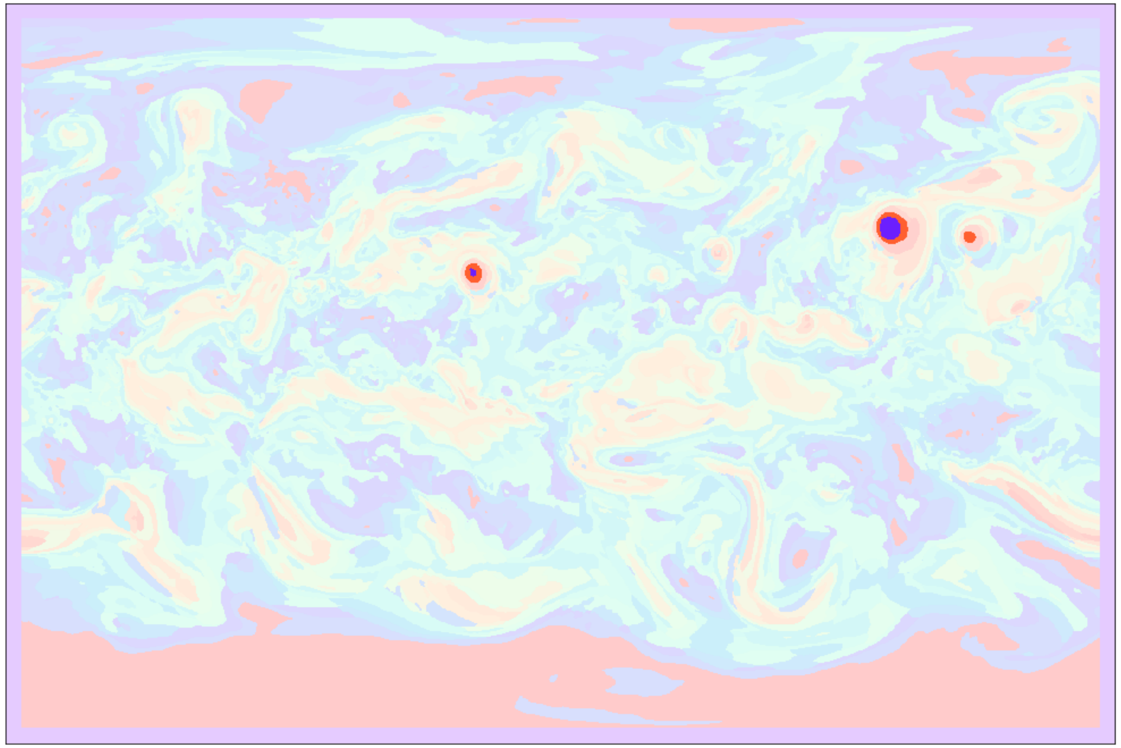
Hurricanes as Coherent Structures

Approximate (local) causal states of Integrated Vapor Transport field of GCM

A. Rupe et al, DisCo: Physics-based unsupervised discovery of coherent structures in spatiotemporal systems. IEEE/ACM MLHPC Workshop (2019)

Isolate states corresponding to hurricanes





Transfer Operators

- Classical analogs of Quantum (Hilbert space) dynamics
- Dynamical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ with $\omega_t = \Phi^t(\omega_0), \quad \omega \in \Omega$
- *Perron-Frobenius Operator* (Schrödinger picture) — evolves distributions

$$\rho_t(\omega) = P^t \rho, \qquad \rho \in L^1(\Omega, \nu), \quad \rho \geq 0, \quad ||\rho|| = 1$$

- *Koopman Operator* (Heisenberg picture) — evolves observables

$$f_t(\omega) = U^t f = f \circ \Phi^t, \qquad f \in L^\infty(\Omega, \nu)$$

- Both are (semigroups of) *linear, infinite-dimensional* Markov operators
- Provide *spectral analysis* for *any* nonlinear dynamical system

A. Lasota and M. C. Mackey, Chaos, fractals, and noise: stochastic aspects of dynamics. Vol. 97. Springer Science (2013).

Modes of Organization

- meta-stable states and coherent structures as *almost-invariant sets* $\mathbf{v} \in L^1(\Omega, \nu)$

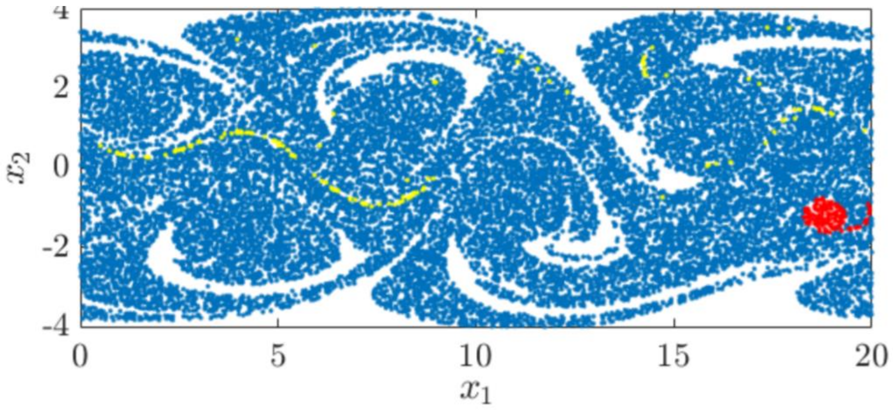
$$P^t \mathbf{v} = \lambda \mathbf{v} \quad \text{with} \quad \lambda \approx 1$$

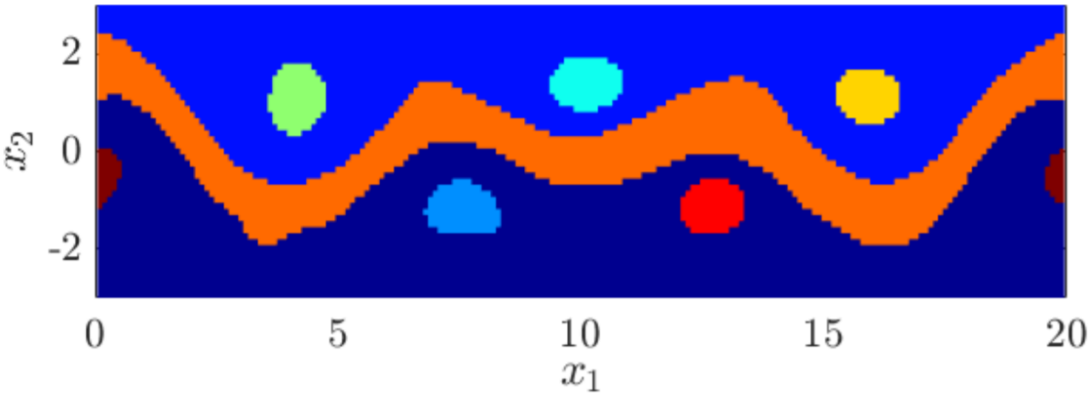
G. Froyland and K. Padberg. Almost-invariant sets and invariant manifolds—connecting probabilistic and geometric descriptions of coherent structures in flows. Physica D (2009)

- decompose identity function ("full-state observable") into *Koopman modes*

$$g(\omega) = \sum_l \eta_l \mathbf{v}_l \quad \text{with} \quad U^t \mathbf{v} = \lambda \mathbf{v}, \quad g(\omega) = \omega$$

M. Budišić, R. Mohr, and I. Mezić. Applied koopmanism. Chaos 22.4 (2012).





S. Klus et al. Kernel methods for detecting coherent structures in dynamical data. Chaos 29.12 (2019)

Nonequilibrium Stat Mech and Partially-Observed Systems

- For Dynamical System $(\Omega, \Sigma_\Omega, \nu, \Phi)$, let $X : \Omega \to \mathcal{X}$ be a non-invertible measurable mapping

- Observations $x_t = X(\omega_t)$ represent *partial information* on state $\omega_t \in \Omega$

  $\implies$ probability space $(\Omega, \Sigma_\Omega, \mu_0)$

- Initial observation $x_0 = X(\omega_0)$ induces uncertainty μ_0 over Ω (e.g. MaxEnt)

- Stochastic process $\{X_t\}$ with r.v.s. $X_t = [U^t X](\omega_0)$ distributed according to (pushforward of) $\mu_t = P^t \mu_0$

- Example, SUS + heat bath: $\omega = (\omega_{SUS}, \omega_{HB})$ and $X(\omega) = \omega_{SUS}$
  evolution $U^t X$ equivalent to tracing out ω_{HB} from $\omega_t = \Phi^t(\omega_0)$

- Can recover 2^{nd} Law in $\{X_t\}$ from Hamiltonian dynamics $(\Omega, \Sigma_\Omega, \nu, \Phi)$
  M. C. Mackey, Time's arrow: The origins of thermodynamic behavior. Springer (1993)

Mori-Zwanzig, Causal States, and Transfer Operators

- Expand U^{t+1} in terms of *projection operator* P (with $Q = I - P$)

$$U^{t+1} = \sum_{k=0}^{t} U^{t-k} PU(QU)^k + (QU)^{t+1}$$

- Apply both sides to observable X: $x_{t+1} = X_{t+1}(\omega_0) = [U^{t+1}X](\omega_0)$
- *Discrete-time MZ equation* (generalized Langevin equation):

$$x_{t+1} = M_0(x_t) + \sum_{k=1}^{t} M_k(x_{t-k}) + \xi_{t+1}(\omega_0)$$

A. J. Chorin, O. H. Hald, and R. Kupferman, Optimal prediction with memory. Physica D (2002)

- Apply both sides to *pasts of observables* $\overleftarrow{X}$: $x_{t+1} = \overleftarrow{M}_0(\overleftarrow{x}_t)$

K. K. Lin and F. Lu, Journal of Computational Physics (2021)   F. Gliani, D. Giannakis, J. Harlim. Physica D (2021)

- one-to-one correspondence between $\overleftarrow{M}_0$ and causal state dynamic M_ϵ

A. Rupe et. al., Learning implicit models of complex dynamical systems from partial observations. in progress (2021)

Thank You!

Thanks to: Jim Crutchfield, Monty Vesselinov, Aric Hagberg, Nicolas Brodu, Derek DeSantis, Stefan Klus, Dan O'Malley, Balu Nadiga, Paul Riechers, Mitko Vassilev

Manuscripts (hopefully) coming soon

- A. Rupe and J. P. Crutchfield, The search for principles of organization
- A. Rupe et al., Learning implicit models of complex dynamical systems from partial observations
- A. Rupe and J. P. Crutchfield, An algebraic theory of patterns as generalized symmetries